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Adsorption of Helium Atoms on Two-Dimensional Substrates

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Abstract

© 2016 Springer Science+Business Media New York The study of the adsorption phenomenon of helium began many decades ago with the discovery of graphite as a homogeneous substrate for the investigation of physically adsorbed monolayer films. In particular, helium monoatomic layers on graphite were found to exhibit a very rich phase diagram. In the present work we have investigated the adsorption phenomenon of helium atoms on graphene and silicene substrates by means of density functional theory with Born–Oppenheimer approximation. Helium–substrate and helium–helium interactions were considered from first principles. Vibrational properties of adsorbed monolayers have been used to explore the stability of the system. This approach reproduces results describing the stability of a helium monolayer on graphene calculated by quantum Monte Carlo (QMC) simulations for low and high coverage cases. However, for the moderate coverage value there is a discrepancy with QMC results due to the lack of helium zero point motion.

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Keywords

Adsorption, Density functional theory, Graphene, Helium, Silicene